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(6) UNUSUAL OXIDATION STATES AND COORDINATION NUMBERS OF THE LIGHT ELEMENTS.

By

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The research under this contract was devoted to the development and testing of quantum mechanical techniques suitable for studying novel geometries, coordination and oxidation states of the light elements. Prediction of stabilities and various aspects of their chemistry was also made for numerous molecular complexes of these elements. In particular, HeF^+, NeF^+, HeO^+, NeO^+, HeN^+, NeN^+, ArO^+, and ArF^+, generally in combination with the counter ions PtF_6^- and SbF_6^-, are expected to show stability in one or several molecular states. The existence of noble gas boron compounds also appears possible under appropriate circumstances.

Three graduate students and one postdoctoral research associate were trained under this contract and two of these have continued in this general area and are themselves currently producing important new chemical information that is certain to aid the mission of ONR.

It is possible to make a general conclusion from the specific research funded by this contract that should be of far reaching significance to ONR. Eventhough none of the particular compounds studied have ended up in fleet usage, a new theoretical capability was demonstrated which is in many ways on an equal footing with traditional experimental techniques and which in some cases may have a decided economic advantage. This new theoretical approach is currently being employed in numerous laboratories and is largely the result of continued advances in applied quantum mechanics and in the revolutionary changes in computer hardware and software. The method is basically "numerical experiments" and as such it is well matched to the subject matter of chemistry and to traditional "instrumental experiments".

Scientific and technical details of the research supported by this contract and acknowledged to it have been reported in the following scientific journal articles:

1. Possible Argon Compounds, J.F. Liebman and L.C. Allen, Chem. Comm. 1355 (1969).

2. Quantum Theory of Structure and Dynamics, L.C. Allen, Ann. Rev. Phys. Chem. 20, 315 (1969).

3. Electronic Structure and Inversion Barrier of Ammonia, A. Rauk, L.C. Allen, and E. Clementi, J. Chem. Phys. 52, 4133 (1970).

4. A Salt Chemistry of Light Noble Gas Compounds, J.F. Liebman and L.C. Allen, J. Amer. Chem. Soc. 92, 3539 (1970).

5. Ab Initio Study of the Geometries Jahn-Teller Distortions, and Electronic Charge Distribution in the CH_4^+ Ion, J. Arents and L.C. Allen, J. Chem. Phys. 53, 73 (1970).

6. Bonding in Rare Gas Diatomic Ions Containing Nitrogen or Oxygen, J.F. Liebman and L.C. Allen, Inter. J. of Mass Spect. and Ion Physics. 7, 27 (1971).

7. Electronic Structure of Carbonium Ions. Methyl and Ethyl Cations. J. E. Williams, V. Buss, and L.C. Allen, J. Amer. Chem. Soc. 93, 6867 (1971).

8. Adequacy of the Molecular Orbital Approximation for Predicting Rotation and Inversion Barriers, L.C. Allen and J. Arents, J. Chem. Phys. 57, 1818 (1972).

9. Singlet-Triplet Energy Separation, Walsh-Mulliken Diagrams, and Singlet d-Polarization Effects in Methylene, C.F. Bender, H.F. Schaefer, D.R. Franceschetti, and L.C. Allen, J. Amer. Chem. Soc. 94, 6888 (1972).

10. Noble Gas - Boron Compounds, J.F. Liebman and L.C. Allen, Inorganic Chemistry 11, 1143 (1972).

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